



HAL
open science

Benzyltriphenylphosphonium dichloridotriphenylstannate(IV)

Bocar Traore, Mouhamadou Sembene Boye, Mamadou Sidibe, Libasse Diop,
Philippe Guionneau

► **To cite this version:**

Bocar Traore, Mouhamadou Sembene Boye, Mamadou Sidibe, Libasse Diop, Philippe Guionneau. Benzyltriphenylphosphonium dichloridotriphenylstannate(IV). *Acta Crystallographica Section E: Structure Reports Online* [2001-2014], 2013, 69 (1), pp.m42. 10.1107/S1600536812049689. hal-00814544

HAL Id: hal-00814544

<https://hal.science/hal-00814544>

Submitted on 28 Jul 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Benzyltriphenylphosphonium dichlorido-triphenylstannate(IV)

Bocar Traore,^a Mouhamadou Sembene Boye,^a Mamadou Sidibe,^a Libasse Diop^{a*} and Philippe Guionneau^b

^aDepartement de Chimie, Faculté des Sciences et Techniques, Université Cheikh, Anta Diop, Dakar, Senegal, and ^bCNRS, Université de Bordeaux, ICMCB, UPR 9048, 87 avenue du Dr A. Schweitzer, F-33608 Pessac, France

Correspondence e-mail: dlibasse@gmail.com

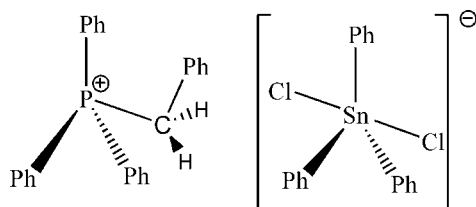
Received 30 September 2012; accepted 3 December 2012

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.039; wR factor = 0.102; data-to-parameter ratio = 22.0.

The crystal structure of the title salt, $(\text{C}_{25}\text{H}_{22}\text{P})[\text{Sn}(\text{C}_6\text{H}_5)_3\text{Cl}_2]$ or $(\text{PhCH}_2\text{PPh}_3)[\text{SnPh}_3\text{Cl}_2]$, consists of $[\text{PhCH}_2\text{PPh}_3]^+$ cations and $[\text{SnPh}_3\text{Cl}_2]^-$ anions in which the Sn^{IV} atom is linked to two Cl atoms and three phenyl groups in a trigonal-bipyramidal geometry, with the Cl atoms in *trans* positions. The cation adopts a tetrahedral geometry. In the crystal, the cations and the anions are connected by $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds, leading to an infinite chain propagating along the c direction.

Related literature

For the $[\text{SnPh}_3\text{Cl}_2]^-$ anion, see: Harrison *et al.* (1978); Ng (1995). For applications of tin based materials, see: Dutrecq *et al.* (1992).



Experimental

Crystal data

$(\text{C}_{25}\text{H}_{22}\text{P})[\text{Sn}(\text{C}_6\text{H}_5)_3\text{Cl}_2]$

$M_r = 774.29$

Monoclinic, $P2_1/c$
 $a = 10.0222$ (2) Å
 $b = 17.1480$ (3) Å
 $c = 21.2925$ (4) Å
 $\beta = 92.042$ (1)°
 $V = 3657.02$ (12) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.92$ mm⁻¹
 $T = 293$ K
 $0.25 \times 0.25 \times 0.25$ mm

Data collection

Nonius KappaCCD diffractometer
 Absorption correction: multi-scan
 (*SCALEPACK*; Otwinowski & Minor, 1997)
 $T_{\text{min}} = 0.803$, $T_{\text{max}} = 0.803$

29025 measured reflections
 9370 independent reflections
 6243 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.072$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.102$
 $S = 1.03$
 9370 reflections

425 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.80$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.76$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| $\text{C}35-\text{H}35\cdots\text{Cl}2$ | 0.93 | 2.94 | 3.696 (3) | 139 |
| $\text{C}37-\text{H}37A\cdots\text{Cl}1^i$ | 0.97 | 2.84 | 3.743 (3) | 155 |
| $\text{C}30-\text{H}30\cdots\text{Cl}1^i$ | 0.93 | 2.67 | 3.596 (3) | 171 |

Symmetry code: (i) $x + 1, -y + \frac{1}{2}, z - \frac{1}{2}$.

Data collection: *COLLECT* (Nonius, 2003); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2448).

References

- Dutrecq, A., Willem, R., Biesemans, M., Bouâlam, M., Meriem, A. & Gielen, M. (1992). *Main Group Met. Chem.* **15**, 285–291.
 Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
 Harrison, P. G., Molloy, K. C., Phillips, R. C., Smith, P. J. & Crowe, A. J. (1978). *J. Organomet. Chem.* **160**, 421–434.
 Ng, S. W. (1995). *Acta Cryst.* **C51**, 1124–1125.
 Nonius (2003). *COLLECT*. Nonius BV, Delft, The Netherlands.
 Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2013). E69, m42 [doi:10.1107/S1600536812049689]

Benzyltriphenylphosphonium dichloridotriphenylstannate(IV)

Bocar Traore, Mouhamadou Sembene Boye, Mamadou Sidibe, Libasse Diop and Philippe Guionneau

Comment

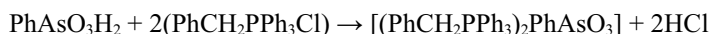
The structure of $[\text{SnPh}_3\text{Cl}_2]^-$ stabilized with different counterions have been reported (Harrison *et al.*, 1978; Ng, 1995). In the scope of our research work toward new organotin (IV) compounds, owing to their various applications: agrochemicals, surface disinfectants, wood preservatives, and marine-antifouling paints (Dutrecq *et al.*, 1992), we report here the crystal structure of $[\text{PhCH}_2\text{PPh}_3][\text{SnPh}_3\text{Cl}_2]$.

In the asymmetric unit of the title compound (Fig. 1), the anion $[\text{SnPh}_3\text{Cl}_2]^-$ adopts a trigonal bipyramidal geometry, the chloride atoms occupy the apical positions while the phenyl groups are equatorial. The Sn—C bonds are [2.135 (3); 2.142 (3); 2.153 (3) Å] while the Sn—Cl distances [2.5795 (7); 2.6127 (7) Å] are very similar to the unique Sn—Cl distance value [2.598 (1) Å] (Ng, 1995) but respectively longer and shorter than those [2.573 (7); 2.689 (6) Å] reported (Harrison *et al.*, 1978) within the same anion. The sum of the equatorial angles (360°) is consistent with almost perfectly planar SnPh_3 residue, while the Cl—Sn—Cl deviates from linearity [$175.77 (3)^\circ$].

$[\text{SnPh}_3\text{Cl}_2]^-$ and $[\text{PhCH}_2\text{PPh}_3]^+$ are linked through short C—H \cdots Cl contacts (Table 1 & Fig. 2).

Experimental

All chemicals were purchased from Aldrich (Germany) and used without any further purification. The studied adduct is obtained following a two stage reaction. Synthesis of $(\text{PhCH}_2\text{PPh}_3)_2\text{PhAsO}_3$: this salt is obtained by neutralization of PhAsO_3H_2 (9.899 mmol in water) by $\text{PhCH}_2\text{PPh}_3\text{Cl}$ (19.798 mmol in ethanolic solution) according to the following reaction:



Synthesis of $[\text{PhCH}_2\text{PPh}_3][\text{SnPh}_3\text{Cl}_2]$: this compound was obtained by mixing ethanolic solutions of $(\text{PhCH}_2\text{PPh}_3)_2\text{PhAsO}_3$ (0.5 mmol) and SnPh_3Cl (1.0 mmol) in a 1/2 ratio. The mixture was stirred for around two hours at room temperature. Suitable crystals for X-ray diffraction were obtained after slow solvent evaporation. (m.p. 393 K). The title compound was isolated according to the following reaction:

**Refinement**

All H atoms were placed in geometrically calculated positions ($d(\text{C—H})=0.93$ Å for phenyl-H and 0.97 Å for methylene-H) and refined using a riding model with $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}$ of the respective carrier atom.

Computing details

Data collection: *COLLECT* (Nonius, 2003); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012);

software used to prepare material for publication: *publCIF* (Westrip, 2010).

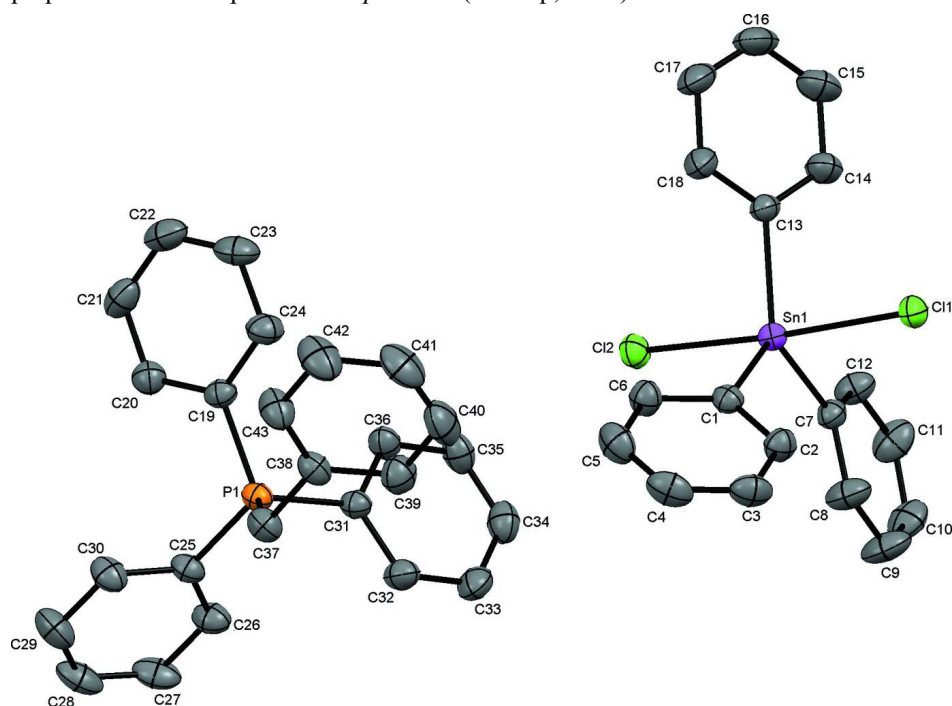


Figure 1

The asymmetric unit of the title compound. Hydrogen atoms have been omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level.

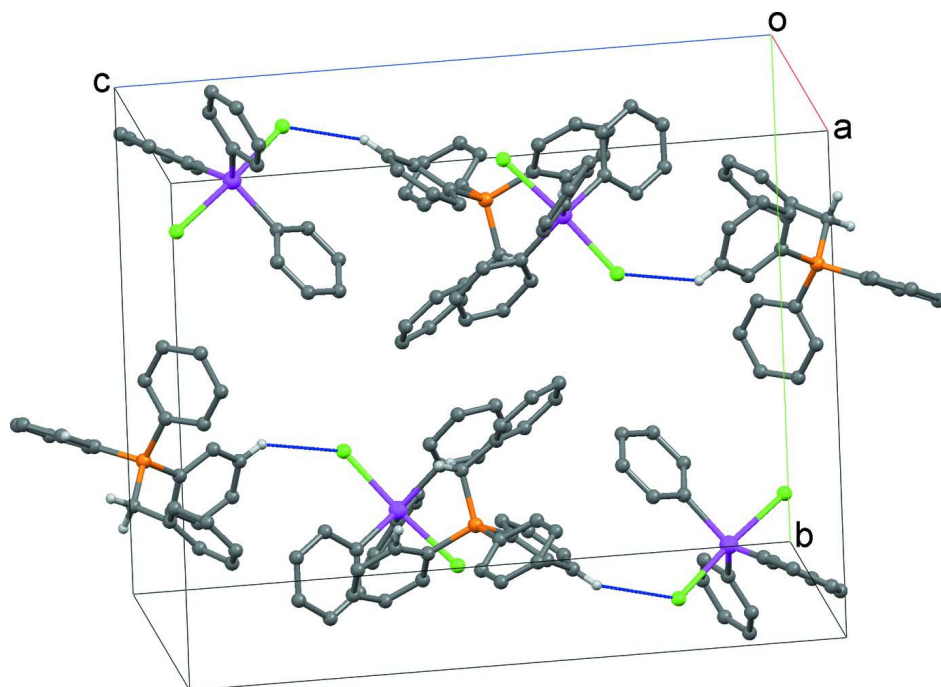


Figure 2

Molecular packing showing hydrogen bonding interactions C—H...Cl (blue lines). H atoms non-participating in hydrogen bonding were omitted for clarity.

Benzyltriphenylphosphonium dichloridotriphenylstannate(IV)

Crystal data

(C₂₅H₂₂P)[Sn(C₆H₅)₃Cl₂]

M_r = 774.29

Monoclinic, *P*2₁/*c*

Hall symbol: -*P* 2ybc

a = 10.0222 (2) Å

b = 17.1480 (3) Å

c = 21.2925 (4) Å

β = 92.042 (1)°

V = 3657.02 (12) Å³

Z = 4

F(000) = 1576

D_x = 1.406 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 57161 reflections

θ = 1.0–28.7°

μ = 0.92 mm⁻¹

T = 293 K

Prism, colorless

0.25 × 0.25 × 0.25 mm

Data collection

Nonius KappaCCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ scans, and ω scans with κ offset

Absorption correction: multi-scan

(*SCALEPACK*; Otwinowski & Minor, 1997)

T_{min} = 0.803, *T_{max}* = 0.803

29025 measured reflections

9370 independent reflections

6243 reflections with *I* > 2σ(*I*)

R_{int} = 0.072

θ_{\max} = 28.6°, θ_{\min} = 1.9°

h = -13→13

k = -23→23

l = -28→24

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.039

wR(*F*²) = 0.102

S = 1.03

9370 reflections

425 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier

map

Hydrogen site location: inferred from

neighbouring sites

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0443*P*)²]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.003

Δρ_{max} = 0.80 e Å⁻³

Δρ_{min} = -0.76 e Å⁻³

Extinction correction: *SHELXS97* (Sheldrick, 2008), *F_c** = *kF_c*[1 + 0.001*xF_c*²λ³/sin(2θ)]^{-1/4}

Extinction coefficient: 0.00069 (19)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of *F*² against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on *F*², conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative *F*². The threshold expression of *F*² > 2σ(*F*²) is used only for calculating *R*-factors(gt) etc. and is not relevant to the choice of reflections for refinement. *R*-factors based on *F*² are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

| | <i>x</i> | <i>y</i> | <i>z</i> | <i>U_{iso}</i> */ <i>U_{eq}</i> |
|-----|---------------|---------------|--------------|---|
| Sn1 | 0.056967 (18) | 0.189828 (11) | 0.831152 (8) | 0.03831 (8) |
| P1 | 0.60102 (8) | 0.16081 (5) | 0.49141 (3) | 0.04170 (18) |
| Cl2 | 0.12400 (8) | 0.07857 (4) | 0.75709 (4) | 0.05285 (19) |

| | | | | |
|------|--------------|--------------|--------------|--------------|
| C11 | -0.00860 (8) | 0.29530 (5) | 0.91305 (4) | 0.05139 (19) |
| C1 | 0.1426 (3) | 0.27746 (17) | 0.77245 (13) | 0.0422 (6) |
| C2 | 0.0886 (3) | 0.35192 (18) | 0.76919 (15) | 0.0514 (7) |
| H2 | 0.0196 | 0.3652 | 0.7952 | 0.062* |
| C6 | 0.2473 (3) | 0.2593 (2) | 0.73420 (15) | 0.0547 (8) |
| H6 | 0.2851 | 0.2098 | 0.7356 | 0.066* |
| C5 | 0.2958 (4) | 0.3156 (2) | 0.69355 (17) | 0.0676 (10) |
| H5 | 0.3669 | 0.3036 | 0.6683 | 0.081* |
| C4 | 0.2394 (4) | 0.3881 (2) | 0.69064 (17) | 0.0684 (10) |
| H4 | 0.2717 | 0.4251 | 0.6631 | 0.082* |
| C3 | 0.1358 (4) | 0.4067 (2) | 0.72789 (16) | 0.0619 (9) |
| H3 | 0.0972 | 0.4559 | 0.7254 | 0.074* |
| C38 | 0.7056 (3) | 0.30371 (17) | 0.53593 (14) | 0.0496 (7) |
| C37 | 0.6618 (3) | 0.25886 (18) | 0.47796 (14) | 0.0507 (7) |
| H37A | 0.7366 | 0.2557 | 0.4504 | 0.061* |
| H37B | 0.5917 | 0.2882 | 0.4560 | 0.061* |
| C43 | 0.8381 (4) | 0.3060 (2) | 0.55450 (17) | 0.0669 (10) |
| H43 | 0.8998 | 0.2784 | 0.5316 | 0.080* |
| C7 | -0.1504 (3) | 0.16911 (17) | 0.81155 (14) | 0.0432 (6) |
| C12 | -0.2192 (3) | 0.1080 (2) | 0.83806 (17) | 0.0599 (9) |
| H12 | -0.1744 | 0.0741 | 0.8656 | 0.072* |
| C8 | -0.2210 (4) | 0.2173 (2) | 0.77078 (19) | 0.0694 (10) |
| H8 | -0.1775 | 0.2590 | 0.7525 | 0.083* |
| C10 | -0.4208 (4) | 0.1446 (2) | 0.7825 (2) | 0.0746 (11) |
| H10 | -0.5105 | 0.1357 | 0.7722 | 0.090* |
| C11 | -0.3545 (4) | 0.0967 (2) | 0.8240 (2) | 0.0748 (11) |
| H11 | -0.3998 | 0.0562 | 0.8430 | 0.090* |
| C13 | 0.1596 (3) | 0.12843 (16) | 0.90599 (13) | 0.0434 (6) |
| C14 | 0.0930 (4) | 0.1035 (2) | 0.95780 (15) | 0.0612 (9) |
| H14 | 0.0025 | 0.1146 | 0.9606 | 0.073* |
| C18 | 0.2933 (3) | 0.1121 (2) | 0.90324 (16) | 0.0621 (9) |
| H18 | 0.3402 | 0.1276 | 0.8685 | 0.074* |
| C39 | 0.6143 (4) | 0.3431 (2) | 0.57196 (17) | 0.0664 (9) |
| H39 | 0.5235 | 0.3409 | 0.5614 | 0.080* |
| C42 | 0.8818 (4) | 0.3480 (3) | 0.60595 (19) | 0.0879 (14) |
| H42 | 0.9721 | 0.3490 | 0.6175 | 0.106* |
| C17 | 0.3594 (4) | 0.0720 (3) | 0.9525 (2) | 0.0814 (12) |
| H17 | 0.4506 | 0.0623 | 0.9510 | 0.098* |
| C15 | 0.1576 (4) | 0.0626 (2) | 1.00562 (18) | 0.0780 (11) |
| H15 | 0.1102 | 0.0458 | 1.0398 | 0.094* |
| C16 | 0.2897 (5) | 0.0469 (2) | 1.00310 (19) | 0.0824 (12) |
| H16 | 0.3330 | 0.0193 | 1.0354 | 0.099* |
| C9 | -0.3557 (4) | 0.2053 (3) | 0.7564 (2) | 0.0876 (13) |
| H9 | -0.4013 | 0.2388 | 0.7288 | 0.105* |
| C40 | 0.6596 (5) | 0.3860 (2) | 0.62403 (19) | 0.0838 (13) |
| H40 | 0.5990 | 0.4131 | 0.6479 | 0.101* |
| C41 | 0.7921 (5) | 0.3884 (3) | 0.64018 (19) | 0.0862 (13) |
| H41 | 0.8217 | 0.4177 | 0.6747 | 0.103* |
| C31 | 0.4480 (3) | 0.16491 (17) | 0.53283 (13) | 0.0420 (6) |

| | | | | |
|-----|------------|--------------|--------------|-------------|
| C32 | 0.3462 (3) | 0.2142 (2) | 0.51172 (16) | 0.0571 (8) |
| H32 | 0.3594 | 0.2474 | 0.4779 | 0.068* |
| C36 | 0.4276 (3) | 0.11637 (18) | 0.58369 (14) | 0.0507 (7) |
| H36 | 0.4951 | 0.0832 | 0.5984 | 0.061* |
| C34 | 0.2063 (4) | 0.1663 (2) | 0.59126 (18) | 0.0657 (10) |
| H34 | 0.1251 | 0.1670 | 0.6111 | 0.079* |
| C33 | 0.2255 (3) | 0.2142 (2) | 0.54078 (17) | 0.0659 (9) |
| H33 | 0.1569 | 0.2467 | 0.5261 | 0.079* |
| C35 | 0.3058 (4) | 0.1177 (2) | 0.61241 (16) | 0.0620 (9) |
| H35 | 0.2917 | 0.0852 | 0.6465 | 0.074* |
| C25 | 0.5706 (3) | 0.11860 (18) | 0.41469 (13) | 0.0460 (7) |
| C26 | 0.4456 (3) | 0.0926 (2) | 0.39523 (15) | 0.0566 (8) |
| H26 | 0.3747 | 0.0959 | 0.4221 | 0.068* |
| C30 | 0.6763 (3) | 0.1134 (2) | 0.37403 (14) | 0.0582 (8) |
| H30 | 0.7605 | 0.1318 | 0.3863 | 0.070* |
| C27 | 0.4260 (4) | 0.0616 (2) | 0.33573 (17) | 0.0699 (10) |
| H27 | 0.3416 | 0.0447 | 0.3223 | 0.084* |
| C28 | 0.5301 (4) | 0.0557 (2) | 0.29691 (16) | 0.0731 (11) |
| H28 | 0.5161 | 0.0343 | 0.2571 | 0.088* |
| C29 | 0.6545 (4) | 0.0806 (2) | 0.31523 (16) | 0.0710 (10) |
| H29 | 0.7249 | 0.0755 | 0.2882 | 0.085* |
| C19 | 0.7220 (3) | 0.10487 (17) | 0.53669 (14) | 0.0438 (6) |
| C20 | 0.7749 (3) | 0.03695 (19) | 0.51251 (16) | 0.0532 (8) |
| H20 | 0.7490 | 0.0203 | 0.4723 | 0.064* |
| C24 | 0.7603 (3) | 0.1281 (2) | 0.59706 (15) | 0.0580 (8) |
| H24 | 0.7233 | 0.1726 | 0.6142 | 0.070* |
| C21 | 0.8664 (3) | -0.0061 (2) | 0.54841 (19) | 0.0671 (10) |
| H21 | 0.9012 | -0.0521 | 0.5325 | 0.080* |
| C23 | 0.8526 (4) | 0.0853 (2) | 0.63147 (17) | 0.0710 (10) |
| H23 | 0.8792 | 0.1018 | 0.6716 | 0.085* |
| C22 | 0.9059 (4) | 0.0190 (3) | 0.6076 (2) | 0.0727 (11) |
| H22 | 0.9689 | -0.0092 | 0.6312 | 0.087* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Sn1 | 0.03712 (11) | 0.04086 (12) | 0.03680 (11) | 0.00303 (8) | -0.00100 (7) | 0.00082 (8) |
| P1 | 0.0413 (4) | 0.0461 (4) | 0.0374 (4) | -0.0044 (3) | -0.0027 (3) | 0.0008 (3) |
| Cl2 | 0.0652 (5) | 0.0463 (4) | 0.0473 (4) | 0.0065 (4) | 0.0060 (3) | -0.0056 (3) |
| Cl1 | 0.0534 (4) | 0.0544 (4) | 0.0463 (4) | 0.0097 (4) | 0.0002 (3) | -0.0090 (3) |
| C1 | 0.0402 (15) | 0.0449 (15) | 0.0413 (15) | -0.0045 (13) | -0.0026 (12) | -0.0017 (13) |
| C2 | 0.0552 (18) | 0.0433 (17) | 0.0557 (18) | 0.0043 (15) | 0.0008 (14) | -0.0006 (14) |
| C6 | 0.0542 (19) | 0.0526 (19) | 0.0577 (19) | -0.0007 (16) | 0.0095 (15) | 0.0025 (15) |
| C5 | 0.066 (2) | 0.079 (3) | 0.059 (2) | -0.021 (2) | 0.0152 (18) | -0.0001 (18) |
| C4 | 0.089 (3) | 0.058 (2) | 0.058 (2) | -0.027 (2) | -0.0060 (19) | 0.0144 (17) |
| C3 | 0.080 (2) | 0.0432 (17) | 0.061 (2) | -0.0042 (18) | -0.0120 (18) | 0.0099 (16) |
| C38 | 0.0605 (19) | 0.0449 (17) | 0.0435 (16) | -0.0105 (15) | 0.0022 (14) | -0.0030 (13) |
| C37 | 0.0569 (18) | 0.0494 (17) | 0.0461 (17) | -0.0106 (15) | 0.0034 (14) | -0.0005 (14) |
| C43 | 0.056 (2) | 0.083 (3) | 0.062 (2) | -0.0204 (19) | 0.0075 (16) | -0.0217 (19) |
| C7 | 0.0382 (14) | 0.0452 (16) | 0.0459 (16) | 0.0028 (13) | -0.0020 (12) | -0.0035 (13) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C12 | 0.0490 (18) | 0.0528 (19) | 0.077 (2) | -0.0025 (16) | -0.0096 (16) | 0.0087 (17) |
| C8 | 0.0503 (19) | 0.070 (2) | 0.086 (3) | -0.0014 (18) | -0.0163 (18) | 0.025 (2) |
| C10 | 0.0407 (18) | 0.081 (3) | 0.101 (3) | -0.001 (2) | -0.0126 (19) | -0.012 (2) |
| C11 | 0.048 (2) | 0.067 (2) | 0.110 (3) | -0.0116 (19) | 0.001 (2) | 0.004 (2) |
| C13 | 0.0453 (16) | 0.0420 (15) | 0.0424 (15) | 0.0074 (13) | -0.0072 (12) | -0.0028 (13) |
| C14 | 0.062 (2) | 0.070 (2) | 0.0514 (19) | 0.0067 (18) | -0.0014 (15) | 0.0151 (17) |
| C18 | 0.0497 (18) | 0.077 (2) | 0.058 (2) | 0.0162 (18) | -0.0059 (15) | -0.0075 (18) |
| C39 | 0.070 (2) | 0.059 (2) | 0.070 (2) | 0.0042 (19) | 0.0032 (19) | -0.0080 (18) |
| C42 | 0.077 (3) | 0.115 (4) | 0.071 (3) | -0.035 (3) | -0.002 (2) | -0.025 (3) |
| C17 | 0.068 (2) | 0.095 (3) | 0.079 (3) | 0.036 (2) | -0.025 (2) | -0.011 (2) |
| C15 | 0.096 (3) | 0.082 (3) | 0.056 (2) | 0.003 (2) | -0.008 (2) | 0.021 (2) |
| C16 | 0.106 (3) | 0.077 (3) | 0.062 (2) | 0.029 (3) | -0.030 (2) | 0.007 (2) |
| C9 | 0.054 (2) | 0.094 (3) | 0.113 (4) | 0.012 (2) | -0.028 (2) | 0.026 (3) |
| C40 | 0.117 (4) | 0.073 (3) | 0.063 (2) | 0.007 (3) | 0.018 (2) | -0.019 (2) |
| C41 | 0.116 (4) | 0.084 (3) | 0.058 (2) | -0.032 (3) | -0.003 (2) | -0.023 (2) |
| C31 | 0.0397 (15) | 0.0454 (15) | 0.0405 (15) | -0.0030 (13) | -0.0018 (12) | 0.0029 (12) |
| C32 | 0.0489 (18) | 0.067 (2) | 0.0549 (19) | 0.0024 (16) | -0.0030 (14) | 0.0130 (17) |
| C36 | 0.0597 (19) | 0.0452 (17) | 0.0476 (17) | 0.0024 (15) | 0.0076 (14) | 0.0035 (13) |
| C34 | 0.051 (2) | 0.076 (2) | 0.071 (2) | -0.0071 (19) | 0.0140 (17) | -0.015 (2) |
| C33 | 0.0440 (18) | 0.083 (3) | 0.070 (2) | 0.0124 (18) | -0.0071 (16) | -0.007 (2) |
| C35 | 0.074 (2) | 0.056 (2) | 0.057 (2) | -0.0088 (19) | 0.0228 (18) | -0.0001 (16) |
| C25 | 0.0502 (16) | 0.0496 (17) | 0.0378 (15) | -0.0092 (14) | -0.0041 (12) | -0.0003 (13) |
| C26 | 0.0509 (18) | 0.068 (2) | 0.0503 (18) | -0.0128 (17) | -0.0074 (14) | 0.0029 (16) |
| C30 | 0.0579 (19) | 0.068 (2) | 0.0485 (18) | -0.0169 (18) | -0.0013 (15) | -0.0095 (16) |
| C27 | 0.077 (2) | 0.076 (2) | 0.055 (2) | -0.030 (2) | -0.0251 (18) | 0.0039 (18) |
| C28 | 0.107 (3) | 0.070 (2) | 0.0406 (18) | -0.024 (2) | -0.0170 (19) | -0.0041 (17) |
| C29 | 0.091 (3) | 0.080 (3) | 0.0430 (18) | -0.018 (2) | 0.0107 (18) | -0.0062 (18) |
| C19 | 0.0385 (14) | 0.0457 (16) | 0.0468 (16) | -0.0023 (13) | -0.0028 (12) | 0.0033 (13) |
| C20 | 0.0506 (18) | 0.0546 (19) | 0.0543 (18) | -0.0031 (16) | 0.0009 (14) | -0.0032 (15) |
| C24 | 0.063 (2) | 0.059 (2) | 0.0512 (18) | 0.0004 (17) | -0.0140 (15) | -0.0041 (16) |
| C21 | 0.055 (2) | 0.056 (2) | 0.091 (3) | 0.0112 (18) | 0.0097 (19) | 0.014 (2) |
| C23 | 0.069 (2) | 0.083 (3) | 0.058 (2) | -0.009 (2) | -0.0234 (18) | 0.013 (2) |
| C22 | 0.054 (2) | 0.081 (3) | 0.082 (3) | 0.005 (2) | -0.0111 (19) | 0.026 (2) |

Geometric parameters (Å, °)

| | | | |
|---------|------------|---------|-----------|
| Sn1—C7 | 2.135 (3) | C42—C41 | 1.366 (6) |
| Sn1—C13 | 2.142 (3) | C42—H42 | 0.9300 |
| Sn1—C1 | 2.153 (3) | C17—C16 | 1.373 (6) |
| Sn1—Cl2 | 2.5795 (7) | C17—H17 | 0.9300 |
| Sn1—Cl1 | 2.6127 (7) | C15—C16 | 1.354 (6) |
| P1—C31 | 1.797 (3) | C15—H15 | 0.9300 |
| P1—C19 | 1.799 (3) | C16—H16 | 0.9300 |
| P1—C25 | 1.803 (3) | C9—H9 | 0.9300 |
| P1—C37 | 1.814 (3) | C40—C41 | 1.360 (6) |
| C1—C6 | 1.386 (4) | C40—H40 | 0.9300 |
| C1—C2 | 1.388 (4) | C41—H41 | 0.9300 |
| C2—C3 | 1.381 (4) | C31—C36 | 1.387 (4) |
| C2—H2 | 0.9300 | C31—C32 | 1.388 (4) |
| C6—C5 | 1.395 (5) | C32—C33 | 1.378 (4) |

| | | | |
|-------------|-------------|-------------|-----------|
| C6—H6 | 0.9300 | C32—H32 | 0.9300 |
| C5—C4 | 1.368 (5) | C36—C35 | 1.384 (4) |
| C5—H5 | 0.9300 | C36—H36 | 0.9300 |
| C4—C3 | 1.366 (5) | C34—C35 | 1.364 (5) |
| C4—H4 | 0.9300 | C34—C33 | 1.372 (5) |
| C3—H3 | 0.9300 | C34—H34 | 0.9300 |
| C38—C43 | 1.373 (5) | C33—H33 | 0.9300 |
| C38—C39 | 1.390 (5) | C35—H35 | 0.9300 |
| C38—C37 | 1.506 (4) | C25—C26 | 1.380 (4) |
| C37—H37A | 0.9700 | C25—C30 | 1.395 (4) |
| C37—H37B | 0.9700 | C26—C27 | 1.381 (5) |
| C43—C42 | 1.370 (5) | C26—H26 | 0.9300 |
| C43—H43 | 0.9300 | C30—C29 | 1.383 (5) |
| C7—C8 | 1.377 (4) | C30—H30 | 0.9300 |
| C7—C12 | 1.386 (4) | C27—C28 | 1.357 (5) |
| C12—C11 | 1.392 (5) | C27—H27 | 0.9300 |
| C12—H12 | 0.9300 | C28—C29 | 1.362 (5) |
| C8—C9 | 1.389 (5) | C28—H28 | 0.9300 |
| C8—H8 | 0.9300 | C29—H29 | 0.9300 |
| C10—C9 | 1.359 (6) | C19—C20 | 1.386 (4) |
| C10—C11 | 1.361 (6) | C19—C24 | 1.387 (4) |
| C10—H10 | 0.9300 | C20—C21 | 1.386 (5) |
| C11—H11 | 0.9300 | C20—H20 | 0.9300 |
| C13—C18 | 1.372 (4) | C24—C23 | 1.372 (5) |
| C13—C14 | 1.378 (4) | C24—H24 | 0.9300 |
| C14—C15 | 1.379 (5) | C21—C22 | 1.376 (5) |
| C14—H14 | 0.9300 | C21—H21 | 0.9300 |
| C18—C17 | 1.401 (5) | C23—C22 | 1.363 (6) |
| C18—H18 | 0.9300 | C23—H23 | 0.9300 |
| C39—C40 | 1.393 (5) | C22—H22 | 0.9300 |
| C39—H39 | 0.9300 | | |
| | | | |
| C7—Sn1—C13 | 120.13 (11) | C41—C42—H42 | 120.1 |
| C7—Sn1—C1 | 114.09 (11) | C43—C42—H42 | 120.1 |
| C13—Sn1—C1 | 125.74 (11) | C16—C17—C18 | 120.0 (4) |
| C7—Sn1—C12 | 91.73 (8) | C16—C17—H17 | 120.0 |
| C13—Sn1—C12 | 87.85 (8) | C18—C17—H17 | 120.0 |
| C1—Sn1—C12 | 92.49 (8) | C16—C15—C14 | 120.4 (4) |
| C7—Sn1—C11 | 88.83 (8) | C16—C15—H15 | 119.8 |
| C13—Sn1—C11 | 88.24 (8) | C14—C15—H15 | 119.8 |
| C1—Sn1—C11 | 91.11 (8) | C15—C16—C17 | 119.6 (4) |
| C12—Sn1—C11 | 175.77 (3) | C15—C16—H16 | 120.2 |
| C31—P1—C19 | 109.17 (13) | C17—C16—H16 | 120.2 |
| C31—P1—C25 | 109.91 (14) | C10—C9—C8 | 120.0 (4) |
| C19—P1—C25 | 111.14 (14) | C10—C9—H9 | 120.0 |
| C31—P1—C37 | 109.76 (14) | C8—C9—H9 | 120.0 |
| C19—P1—C37 | 110.82 (15) | C41—C40—C39 | 120.4 (4) |
| C25—P1—C37 | 106.01 (14) | C41—C40—H40 | 119.8 |
| C6—C1—C2 | 118.6 (3) | C39—C40—H40 | 119.8 |

| | | | |
|---------------|-----------|-------------|-----------|
| C6—C1—Sn1 | 120.7 (2) | C40—C41—C42 | 120.3 (4) |
| C2—C1—Sn1 | 120.6 (2) | C40—C41—H41 | 119.9 |
| C3—C2—C1 | 121.0 (3) | C42—C41—H41 | 119.9 |
| C3—C2—H2 | 119.5 | C36—C31—C32 | 119.4 (3) |
| C1—C2—H2 | 119.5 | C36—C31—P1 | 120.8 (2) |
| C1—C6—C5 | 119.9 (3) | C32—C31—P1 | 119.7 (2) |
| C1—C6—H6 | 120.1 | C33—C32—C31 | 120.1 (3) |
| C5—C6—H6 | 120.1 | C33—C32—H32 | 120.0 |
| C4—C5—C6 | 120.3 (3) | C31—C32—H32 | 120.0 |
| C4—C5—H5 | 119.9 | C35—C36—C31 | 119.5 (3) |
| C6—C5—H5 | 119.9 | C35—C36—H36 | 120.3 |
| C3—C4—C5 | 120.5 (3) | C31—C36—H36 | 120.3 |
| C3—C4—H4 | 119.8 | C35—C34—C33 | 120.2 (3) |
| C5—C4—H4 | 119.8 | C35—C34—H34 | 119.9 |
| C4—C3—C2 | 119.7 (3) | C33—C34—H34 | 119.9 |
| C4—C3—H3 | 120.1 | C34—C33—C32 | 120.1 (3) |
| C2—C3—H3 | 120.1 | C34—C33—H33 | 119.9 |
| C43—C38—C39 | 118.4 (3) | C32—C33—H33 | 119.9 |
| C43—C38—C37 | 120.1 (3) | C34—C35—C36 | 120.7 (3) |
| C39—C38—C37 | 121.5 (3) | C34—C35—H35 | 119.7 |
| C38—C37—P1 | 115.7 (2) | C36—C35—H35 | 119.7 |
| C38—C37—H37A | 108.4 | C26—C25—C30 | 119.6 (3) |
| P1—C37—H37A | 108.4 | C26—C25—P1 | 121.6 (2) |
| C38—C37—H37B | 108.4 | C30—C25—P1 | 118.7 (2) |
| P1—C37—H37B | 108.4 | C25—C26—C27 | 119.8 (3) |
| H37A—C37—H37B | 107.4 | C25—C26—H26 | 120.1 |
| C42—C43—C38 | 121.6 (4) | C27—C26—H26 | 120.1 |
| C42—C43—H43 | 119.2 | C29—C30—C25 | 119.3 (3) |
| C38—C43—H43 | 119.2 | C29—C30—H30 | 120.3 |
| C8—C7—C12 | 117.3 (3) | C25—C30—H30 | 120.3 |
| C8—C7—Sn1 | 119.9 (2) | C28—C27—C26 | 120.0 (3) |
| C12—C7—Sn1 | 122.8 (2) | C28—C27—H27 | 120.0 |
| C7—C12—C11 | 120.8 (3) | C26—C27—H27 | 120.0 |
| C7—C12—H12 | 119.6 | C27—C28—C29 | 121.2 (3) |
| C11—C12—H12 | 119.6 | C27—C28—H28 | 119.4 |
| C7—C8—C9 | 121.6 (4) | C29—C28—H28 | 119.4 |
| C7—C8—H8 | 119.2 | C28—C29—C30 | 120.0 (3) |
| C9—C8—H8 | 119.2 | C28—C29—H29 | 120.0 |
| C9—C10—C11 | 119.9 (4) | C30—C29—H29 | 120.0 |
| C9—C10—H10 | 120.1 | C20—C19—C24 | 119.2 (3) |
| C11—C10—H10 | 120.1 | C20—C19—P1 | 120.6 (2) |
| C10—C11—C12 | 120.3 (4) | C24—C19—P1 | 120.2 (2) |
| C10—C11—H11 | 119.8 | C21—C20—C19 | 119.8 (3) |
| C12—C11—H11 | 119.8 | C21—C20—H20 | 120.1 |
| C18—C13—C14 | 118.2 (3) | C19—C20—H20 | 120.1 |
| C18—C13—Sn1 | 120.8 (2) | C23—C24—C19 | 120.1 (3) |
| C14—C13—Sn1 | 120.9 (2) | C23—C24—H24 | 120.0 |
| C13—C14—C15 | 121.4 (3) | C19—C24—H24 | 120.0 |
| C13—C14—H14 | 119.3 | C22—C21—C20 | 120.1 (4) |

| | | | |
|-----------------|------------|-----------------|------------|
| C15—C14—H14 | 119.3 | C22—C21—H21 | 120.0 |
| C13—C18—C17 | 120.3 (3) | C20—C21—H21 | 120.0 |
| C13—C18—H18 | 119.8 | C22—C23—C24 | 120.8 (4) |
| C17—C18—H18 | 119.8 | C22—C23—H23 | 119.6 |
| C38—C39—C40 | 119.6 (4) | C24—C23—H23 | 119.6 |
| C38—C39—H39 | 120.2 | C23—C22—C21 | 120.0 (4) |
| C40—C39—H39 | 120.2 | C23—C22—H22 | 120.0 |
| C41—C42—C43 | 119.7 (4) | C21—C22—H22 | 120.0 |
| | | | |
| C7—Sn1—C1—C6 | -119.9 (3) | C13—C18—C17—C16 | 1.8 (6) |
| C13—Sn1—C1—C6 | 62.3 (3) | C13—C14—C15—C16 | 1.0 (6) |
| Cl2—Sn1—C1—C6 | -26.9 (3) | C14—C15—C16—C17 | 0.0 (7) |
| Cl1—Sn1—C1—C6 | 150.9 (2) | C18—C17—C16—C15 | -1.4 (7) |
| C7—Sn1—C1—C2 | 56.0 (3) | C11—C10—C9—C8 | 1.5 (7) |
| C13—Sn1—C1—C2 | -121.8 (2) | C7—C8—C9—C10 | -0.2 (7) |
| Cl2—Sn1—C1—C2 | 149.0 (2) | C38—C39—C40—C41 | -1.0 (6) |
| Cl1—Sn1—C1—C2 | -33.2 (2) | C39—C40—C41—C42 | -0.9 (7) |
| C6—C1—C2—C3 | 1.4 (5) | C43—C42—C41—C40 | 1.1 (7) |
| Sn1—C1—C2—C3 | -174.7 (3) | C19—P1—C31—C36 | -12.8 (3) |
| C2—C1—C6—C5 | -0.1 (5) | C25—P1—C31—C36 | 109.3 (3) |
| Sn1—C1—C6—C5 | 175.9 (3) | C37—P1—C31—C36 | -134.4 (3) |
| C1—C6—C5—C4 | -0.9 (6) | C19—P1—C31—C32 | 170.6 (3) |
| C6—C5—C4—C3 | 0.7 (6) | C25—P1—C31—C32 | -67.2 (3) |
| C5—C4—C3—C2 | 0.6 (6) | C37—P1—C31—C32 | 49.0 (3) |
| C1—C2—C3—C4 | -1.6 (5) | C36—C31—C32—C33 | -0.7 (5) |
| C43—C38—C37—P1 | 96.7 (3) | P1—C31—C32—C33 | 175.9 (3) |
| C39—C38—C37—P1 | -83.0 (4) | C32—C31—C36—C35 | 0.2 (5) |
| C31—P1—C37—C38 | 66.4 (3) | P1—C31—C36—C35 | -176.3 (3) |
| C19—P1—C37—C38 | -54.3 (3) | C35—C34—C33—C32 | -0.9 (6) |
| C25—P1—C37—C38 | -174.9 (2) | C31—C32—C33—C34 | 1.0 (6) |
| C39—C38—C43—C42 | -2.2 (6) | C33—C34—C35—C36 | 0.5 (6) |
| C37—C38—C43—C42 | 178.2 (4) | C31—C36—C35—C34 | -0.1 (5) |
| C13—Sn1—C7—C8 | 169.3 (3) | C31—P1—C25—C26 | -1.8 (3) |
| C1—Sn1—C7—C8 | -8.7 (3) | C19—P1—C25—C26 | 119.1 (3) |
| Cl2—Sn1—C7—C8 | -102.2 (3) | C37—P1—C25—C26 | -120.4 (3) |
| Cl1—Sn1—C7—C8 | 82.0 (3) | C31—P1—C25—C30 | 177.3 (3) |
| C13—Sn1—C7—C12 | -11.1 (3) | C19—P1—C25—C30 | -61.8 (3) |
| C1—Sn1—C7—C12 | 171.0 (2) | C37—P1—C25—C30 | 58.7 (3) |
| Cl2—Sn1—C7—C12 | 77.5 (3) | C30—C25—C26—C27 | 0.0 (5) |
| Cl1—Sn1—C7—C12 | -98.4 (3) | P1—C25—C26—C27 | 179.1 (3) |
| C8—C7—C12—C11 | -0.4 (5) | C26—C25—C30—C29 | -1.4 (5) |
| Sn1—C7—C12—C11 | 180.0 (3) | P1—C25—C30—C29 | 179.5 (3) |
| C12—C7—C8—C9 | -0.3 (6) | C25—C26—C27—C28 | 1.0 (6) |
| Sn1—C7—C8—C9 | 179.3 (3) | C26—C27—C28—C29 | -0.6 (6) |
| C9—C10—C11—C12 | -2.2 (7) | C27—C28—C29—C30 | -0.8 (6) |
| C7—C12—C11—C10 | 1.7 (6) | C25—C30—C29—C28 | 1.8 (6) |
| C7—Sn1—C13—C18 | 150.4 (2) | C31—P1—C19—C20 | 118.8 (2) |
| C1—Sn1—C13—C18 | -31.9 (3) | C25—P1—C19—C20 | -2.5 (3) |
| Cl2—Sn1—C13—C18 | 59.6 (3) | C37—P1—C19—C20 | -120.1 (2) |

| | | | |
|-----------------|------------|-----------------|------------|
| C11—Sn1—C13—C18 | -122.0 (3) | C31—P1—C19—C24 | -59.2 (3) |
| C7—Sn1—C13—C14 | -28.9 (3) | C25—P1—C19—C24 | 179.4 (2) |
| C1—Sn1—C13—C14 | 148.8 (2) | C37—P1—C19—C24 | 61.8 (3) |
| C12—Sn1—C13—C14 | -119.6 (3) | C24—C19—C20—C21 | -1.0 (5) |
| C11—Sn1—C13—C14 | 58.7 (3) | P1—C19—C20—C21 | -179.0 (2) |
| C18—C13—C14—C15 | -0.6 (5) | C20—C19—C24—C23 | 2.0 (5) |
| Sn1—C13—C14—C15 | 178.7 (3) | P1—C19—C24—C23 | -179.9 (3) |
| C14—C13—C18—C17 | -0.9 (5) | C19—C20—C21—C22 | -0.8 (5) |
| Sn1—C13—C18—C17 | 179.9 (3) | C19—C24—C23—C22 | -1.3 (6) |
| C43—C38—C39—C40 | 2.4 (5) | C24—C23—C22—C21 | -0.5 (6) |
| C37—C38—C39—C40 | -177.9 (3) | C20—C21—C22—C23 | 1.5 (6) |
| C38—C43—C42—C41 | 0.4 (7) | | |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------------|-------|-------------|-------------|---------------|
| C35—H35 \cdots C12 | 0.93 | 2.94 | 3.696 (3) | 139 |
| C37—H37A \cdots C11 ⁱ | 0.97 | 2.84 | 3.743 (3) | 155 |
| C30—H30 \cdots C11 ⁱ | 0.93 | 2.67 | 3.596 (3) | 171 |

Symmetry code: (i) $x+1, -y+1/2, z-1/2$.